This dataset contains:

Analytical characterisation of the new ligands and complexes (CHN microanalysis).

^{1}H and ^{13}C NMR spectra of the new organic ligands (raw data).

Paramagnetic ^{1}H NMR spectra of the iron complexes (raw data).

X-ray Crystallographic data:

- Structure of bpp^{COOH} (CCDC 1844095).
- Structure of L^{1} (CCDC 1844096).
- Structure of L^{2} (CCDC 1844097).
- Structure of $L^{3}C_{12}$ (CCDC 1844098).
- Structure of $L^{3}C_{14}$ (CCDC 1854266).
- Structure of $L^{4}C_{12}$ (CCDC 1844099).
- Structure of $[Fe(L^{1})_{2}][BF_{4}]_{2}$ (CCDC 1844100).
- Structure of $[Fe(L^{2})_{2}][BF_{4}]_{2}$ (CCDC 1844101).
- Structure of $[Fe(L^{3}C_{6})_{2}][BF_{4}]_{2}\cdot H_{2}O$ (CCDC 1844102).
- Structure of $[Fe(L^{3}C_{14})_{2}][BF_{4}]_{2}\cdot 2CH_{3}CN$ (CCDC 1854267).
- Structure of $[Fe(L^{3}C_{16})_{2}][BF_{4}]_{2}\cdot H_{2}O$ (CCDC 1844103).

Solid state magnetic susceptibility measurements (raw and processed data).

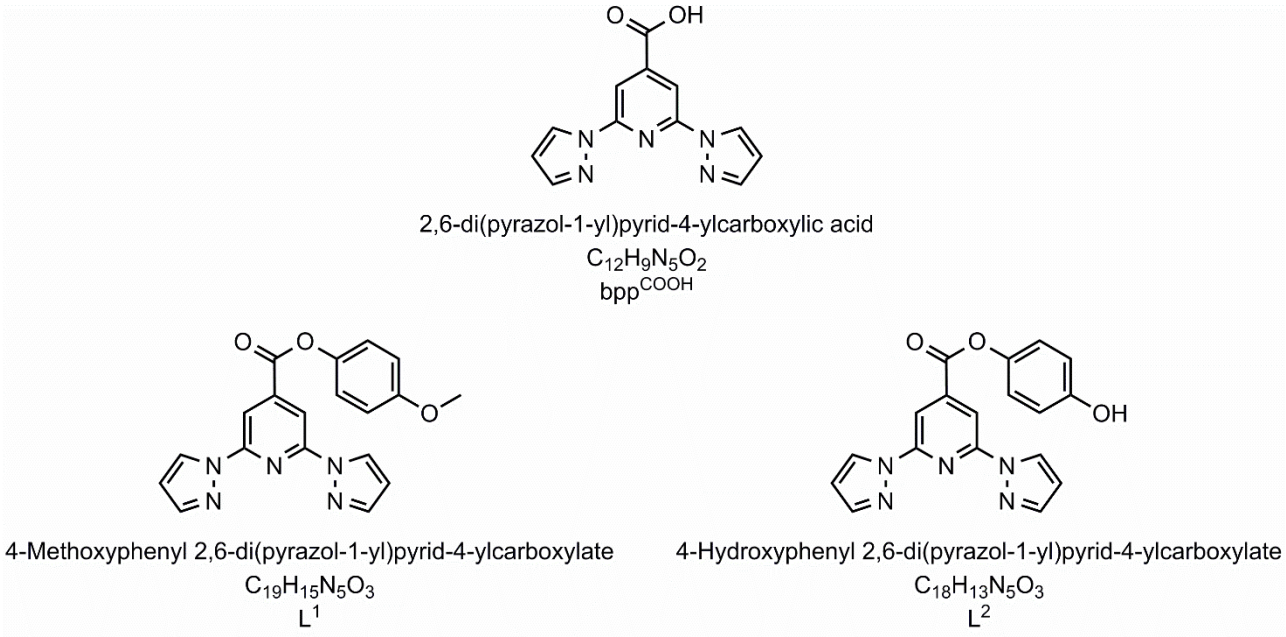
Solution phase magnetic susceptibility measurements (NMR spectra and processed data)

X-ray powder diffraction data (measured and simulated).

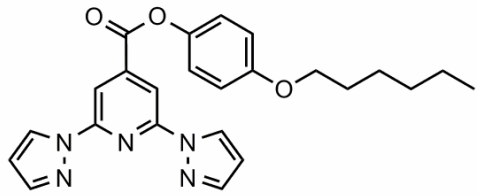
Thermogravimetric analysis (TGA) data.

Differential scanning calorimetry (DSC) data.

Ligands employed in this study



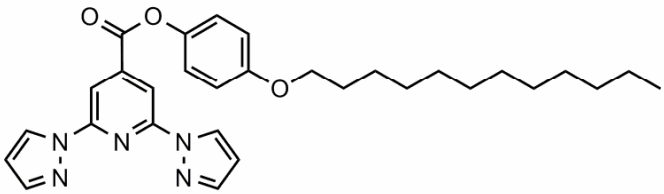
Ligands employed in this study (continued)



4-Hexoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{24}H_{25}N_5O_3$

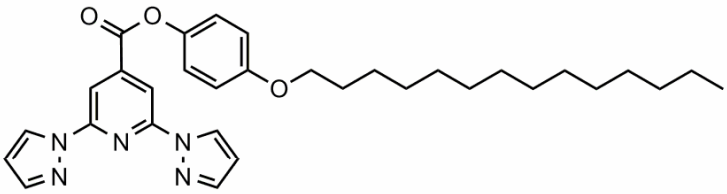
L^3C_6



4-Dodecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{30}H_{37}N_5O_3$

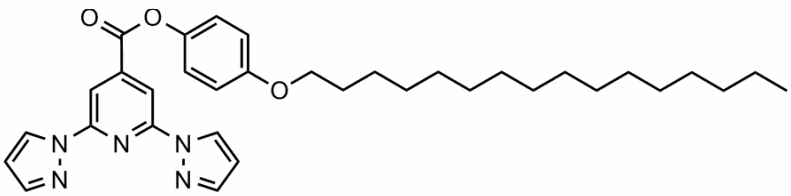
L^3C_{12}



4-Tetradecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{32}H_{41}N_5O_3$

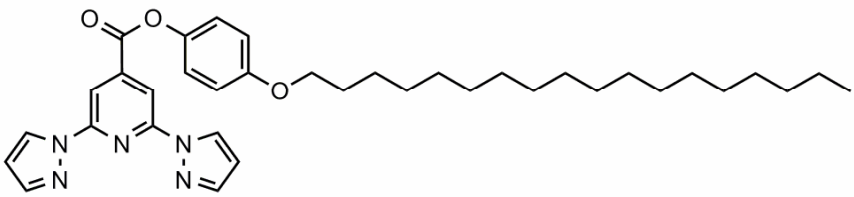
L^3C_{14}



4-Hexadecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{34}H_{45}N_5O_3$

L^3C_{16}

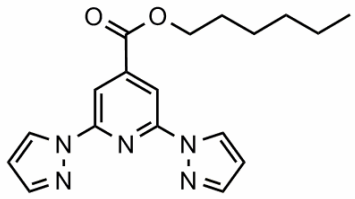


4-Octadecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{36}H_{49}N_5O_3$

L^3C_{18}

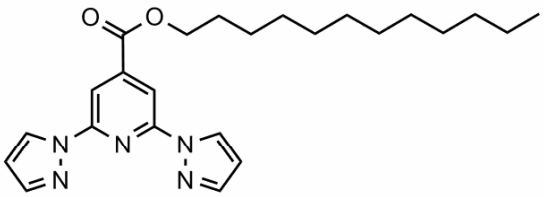
Ligands employed in this study (continued)



Hexyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{18}H_{21}N_5O_3$

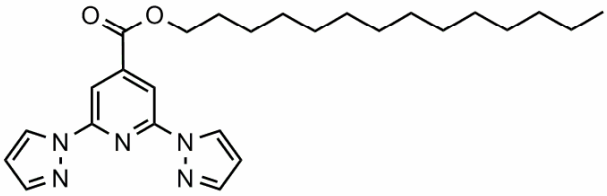
L^4C_6



Dodecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{24}H_{33}N_5O_2$

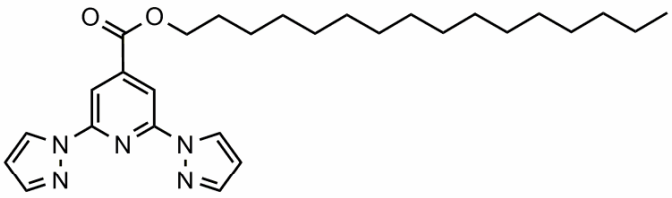
L^4C_{12}



Tetradecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{26}H_{37}N_5O_2$

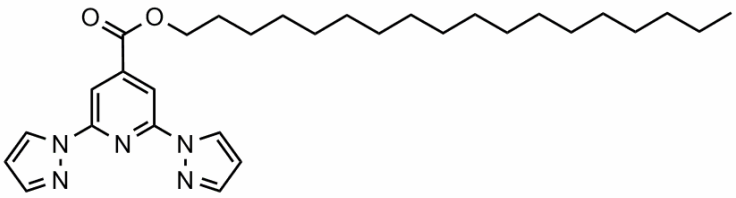
L^4C_{14}



Hexadecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

$C_{28}H_{41}N_5O_2$

L^4C_{16}

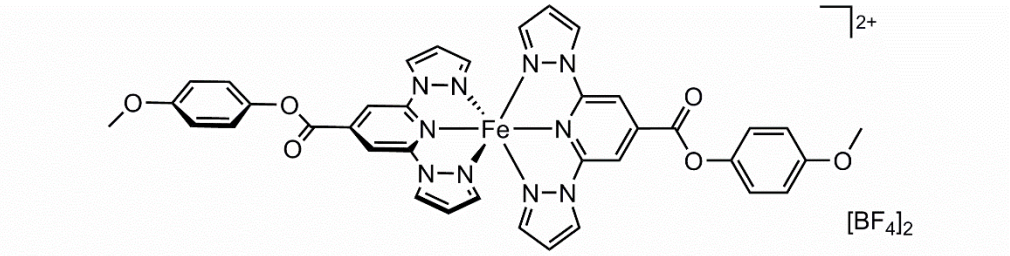


Octadecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate

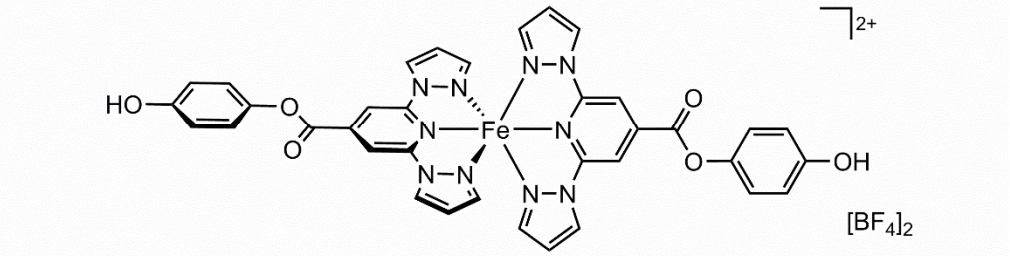
$C_{30}H_{45}N_5O_2$

L^4C_{18}

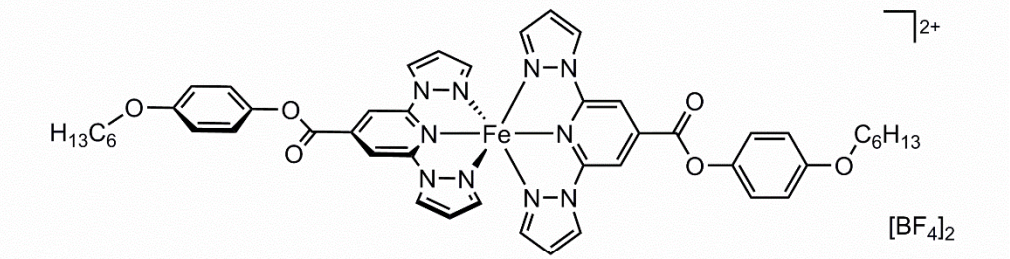
Iron complexes prepared during this study



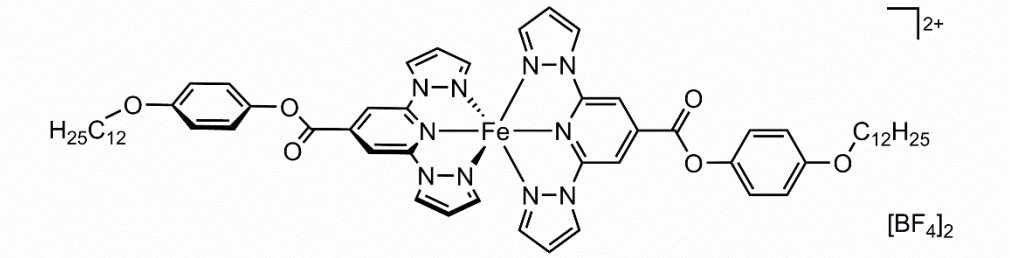
Bis[4-methoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate
$C_{38}H_{30}B_2F_8FeN_{10}O_6$
$[Fe(L^1)_2][BF_4]_2$



Bis[4-hydroxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate
$C_{36}H_{26}B_2F_8FeN_{10}O_6$
$[Fe(L^2)_2][BF_4]_2$

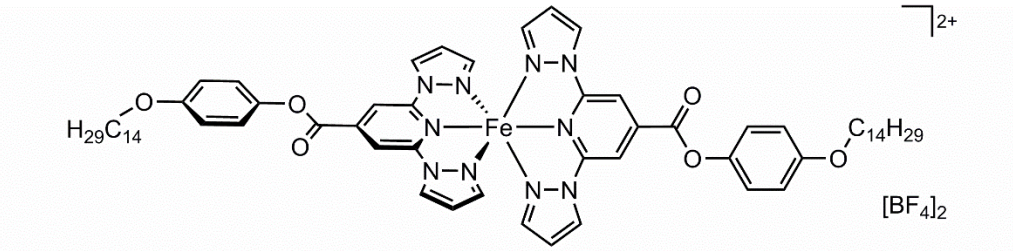


Bis[4-hexoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate
$C_{48}H_{50}B_2F_8FeN_{10}O_6$
$[Fe(L^3C_6)_2][BF_4]_2$



Bis[4-dodecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate
$C_{60}H_{74}B_2F_8FeN_{10}O_6$
$[Fe(L^3C_{12})_2][BF_4]_2$

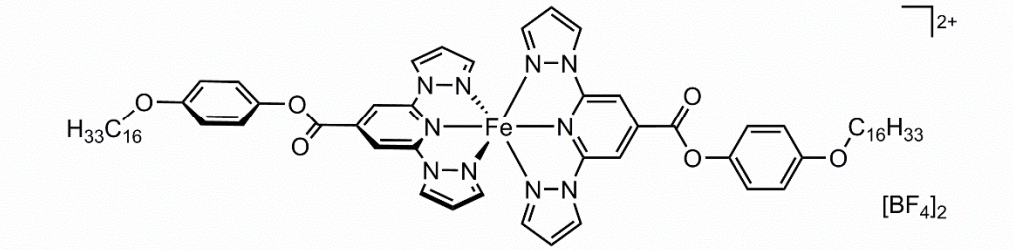
Iron complexes prepared during this study (continued)



Bis[4-tetradecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate

$C_{64}H_{82}B_2F_8FeN_{10}O_6$

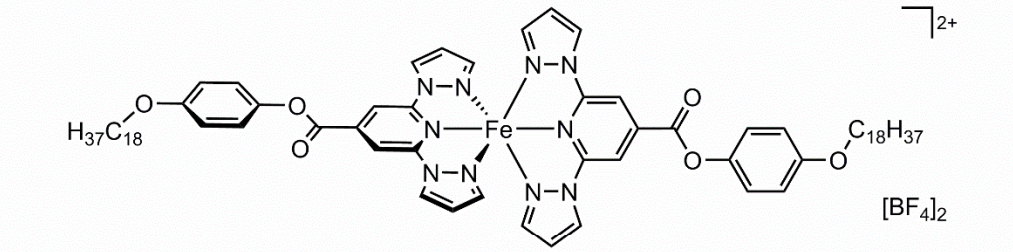
$[Fe(L^3C_{14})_2][BF_4]_2$



Bis[4-hexadecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate

$C_{68}H_{90}B_2F_8FeN_{10}O_6$

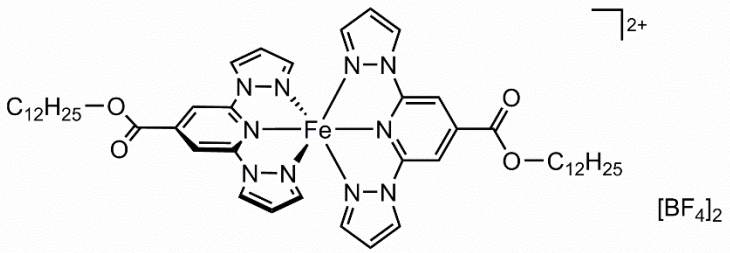
$[Fe(L^3C_{16})_2][BF_4]_2$



Bis[4-octadecoxyphenyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate

$C_{72}H_{98}B_2F_8FeN_{10}O_6$

$[Fe(L^3C_{18})_2][BF_4]_2$

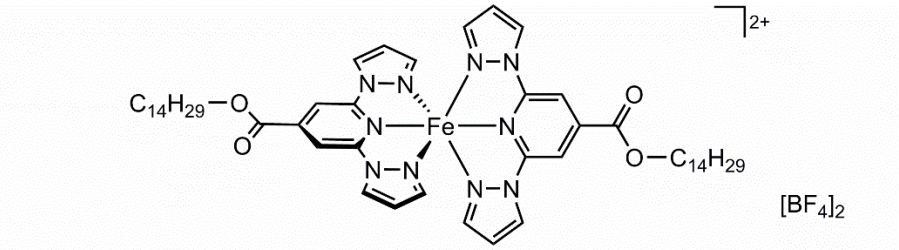


Bis[dodecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate

$C_{48}H_{66}B_2F_8FeN_{10}O_4$

$[Fe(L^4C_{12})_2][BF_4]_2$

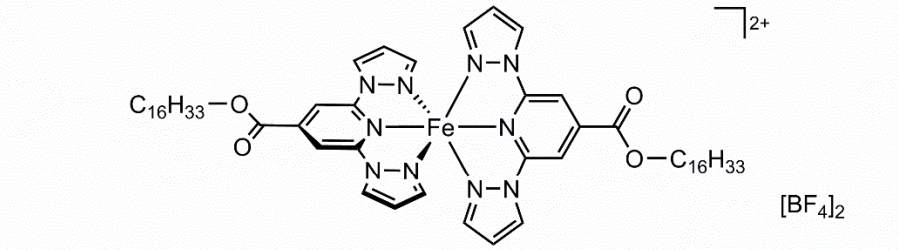
Iron complexes prepared during this study (continued)



Bis[tetradecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate

$C_{52}H_{74}B_2F_8FeN_{10}O_4$

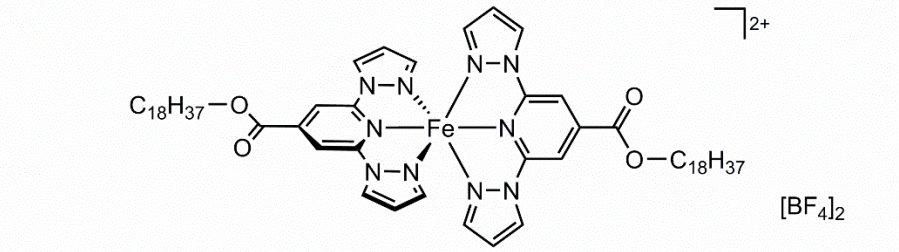
$[Fe(L^4C_{14})_2][BF_4]_2$



Bis[hexadecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate

$C_{56}H_{82}B_2F_8FeN_{10}O_4$

$[Fe(L^4C_{16})_2][BF_4]_2$



Bis[octadecyl 2,6-di(pyrazol-1-yl)pyrid-4-ylcarboxylate]iron(II) di-tetrafluoroborate

$C_{60}H_{90}B_2F_8FeN_{10}O_4$

$[Fe(L^4C_{18})_2][BF_4]_2$